INFRARED SPECTROSCOPY OF WATER CLUSTER RADICAL CATIONS $(H_2O)_n{}^+$ (n = 3 to 11)

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To obtain structural information about radical cationic hydrogen-bonded water networks, we have measured size-selected infrared spectra of the water cluster cations $(H_2O)_n{}^+$ (n = 3–11) in the OH stretching region. The spectra of smaller-sized clusters ($n \leq 6$) show a free OH band associated with the OH radical. This band indicates that nominal water cluster cations $(H_2O)_n{}^+$ form $H^+(H_2O)_{n-1}OH$ type structures, and that the OH radical lies in the network terminal. For larger-sized clusters, the analyses of the hydrogen-bonded OH stretching bands aided by quantum chemical calculations evidence the existence of the OH radical in the clusters. Detailed cluster structures will be discussed on the basis of the experimental spectra.